



Fermi National Accelerator Laboratory

FERMILAB-PUB-95/199-T
July, 1995

Lattice QCD on Small Computers

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July 7, 1995

Abstract

We demonstrate that lattice QCD calculations can be made 10^3 – 10^6 times faster by using very coarse lattices. To obtain accurate results, we replace the standard lattice actions by perturbatively-improved actions with tadpole-improved correction terms that remove the leading errors due to the lattice. To illustrate the power of this approach, we calculate the static-quark potential, and the charmonium spectrum and wavefunctions using a desktop computer. We obtain accurate results that are independent of the lattice spacing and agree well with experiment.



1 Introduction

For 20 years, quantum chromodynamics (QCD) has been the generally accepted theory of strong interactions in particle physics. However, physicists are only just beginning to show that it explains basic features of low-energy strong-interaction physics, such as the spectrum and structure of the hadrons. The most significant progress in the study of low-energy (nonperturbative) QCD has come from numerical simulations of a lattice approximation to the theory. However this approach has been severely limited by the rapid rise in computational difficulty as one approaches the physically relevant limit of small lattice spacing and large lattice volume. In particular the cost of lattice simulations typically grows as a^{-6} when the lattice spacing a is reduced. With standard lattice techniques, it is widely felt that lattice spacings of 0.05–0.1 fm or less are necessary for reasonable accuracy, making simulations impossible on all but the largest computers. In this paper, we suggest modifications of lattice QCD that permit accurate simulations at lattice spacings as large as 0.4 fm, increasing the speed of simulations by a factor of 10^3 – 10^6 . We illustrate our approach with state-of-the-art calculations of the static-quark potential and the charmonium spectrum performed on a high-performance personal computer [1].

The central approximation in lattice QCD is replacing continuous spacetime by a discrete lattice. The QCD action is discretized by replacing space-time integrals with sums and derivatives with differences. Then the path integral defining the field theory can be evaluated numerically using Monte Carlo techniques. Standard discretizations of the QCD action have errors of $\mathcal{O}(a^2)$ that are large when the lattice spacing is 0.4 fm. However improved discretizations can be designed in which finite- a errors are systematically removed by introducing new (nonrenormalizable) interactions into the lattice action. This does not add new parameters to the theory, since the coefficients of the new interactions are determined, from first principles, by demanding that the discretized action reproduces continuum physics to a given accuracy. Since the new interaction terms correct for deficiencies in the short-distance behavior of the lattice theory, their coefficients can be computed using perturbation theory in asymptotically free theories such as QCD, provided the lattice spacing is small enough that perturbation theory is applicable at distances of order a and smaller.

The use of perturbatively improved actions for lattice QCD was suggested

long ago [2]. However early tests showed little benefit from the improvements. Furthermore a variety of studies seemed to indicate that perturbative dynamics was only relevant at distances significantly smaller than 0.1 fm, suggesting that lattice spacings would have to be smaller as well. Recent work [3] on lattice perturbation theory, however, has completely changed this conclusion. If conventional lattice perturbation theory (in terms of the bare coupling) is replaced by an expansion in terms of a renormalized coupling, perturbation theory becomes useful even at distances as large as 0.5 fm. If in addition lattice operators are “tadpole improved” the convergence of the perturbative expansions needed to define improved actions is greatly enhanced. Indeed, as we show here, tree-level calculations of the improvements suffice in most cases provided operators are tadpole-improved. Without tadpole improvement, the correction terms are systematically underestimated, sometimes by factors of two or three.

Tadpole improvement is a technique for summing to all orders the large perturbative contributions that arise from tadpole diagrams peculiar to lattice QCD. At tree level the improvement is trivial to implement: one replaces each lattice QCD link operator U_μ in the action by $\tilde{U}_\mu = U_\mu/u_0$, where u_0 is a scalar mean value of the link, defined to be the fourth root of the expectation value of the four-link plaquette in Monte-Carlo simulations [3].

In several earlier papers, we have advocated the use of perturbatively improved actions with tadpole improvement [1, 3, 4, 5]. Such actions have already proven very successful in simulations of heavy-quark mesons like the Υ . In the nonrelativistic NRQCD quark action [6], both relativistic effects and finite- a corrections are introduced through nonrenormalizable corrections to the basic action. The detailed simulation results presented in [6] agree well with experiment, and many depend crucially on these corrections. Tadpole improvement was essential to this success; test simulations without tadpole improvement underestimated relativistic effects by as much as a factor of two. Similar results have been obtained with improved versions of the Wilson quark action when applied to heavy-quark mesons [7].

In this paper we present new evidence that perturbatively-improved actions, once they are tadpole improved, work well for gluons as well, even at spacings as large as $a = 0.4$ fm. Using improved actions for the quarks and gluons on a lattice with $a = 0.4$ fm, we obtain a static potential that is rotationally invariant to within a few percent, the spin-averaged charmonium spectrum accurate to within 30–40 MeV, and rotationally

invariant charmonium wavefunctions. Our results show lattice-spacing independence (scaling) to within 3%.

2 The Improved Action

The standard Wilson action for gluons has finite- a errors of order a^2 . On coarse lattices these lattice artifacts lead to severe (up to 40%) deviations from rotational invariance of the static quark potential. This can be seen clearly in Fig. 1a (the potential computed on a lattice with $a \approx 0.4$ fm), where the points for $r/a = \sqrt{2}$ and $\sqrt{3}$ lie far off the line defined by $r/a = 1, 2, 3$. These artifacts arise because the plaquette operator, from which the Wilson action is constructed, contains $\mathcal{O}(a^2)$ terms beyond the desired gluon kinetic term when it is expanded in powers of derivatives of the gauge field [8]:

$$1 - \frac{1}{3} \text{Re Tr} U_{\text{pl}} = r_0^{(\text{pl})} \sum_{\mu, \nu} \text{Tr}(F_{\mu\nu} F_{\mu\nu}) + a^2 [r_1^{(\text{pl})} R_1 + r_2^{(\text{pl})} R_2 + r_3^{(\text{pl})} R_3] + \mathcal{O}(a^4) + \text{total derivatives}, \quad (1)$$

where

$$\begin{aligned} R_1 &= \sum_{\mu, \nu} \text{Tr}(D_\mu F_{\mu\nu} D_\mu F_{\mu\nu}), \\ R_2 &= \sum_{\mu, \nu, \sigma} \text{Tr}(D_\mu F_{\nu\sigma} D_\mu F_{\nu\sigma}), \\ R_3 &= \sum_{\mu, \nu, \sigma} \text{Tr}(D_\mu F_{\mu\sigma} D_\nu F_{\nu\sigma}). \end{aligned} \quad (2)$$

Here the r_i are coefficients in the operator product expansion of the plaquette. (Tree-level r_i 's are tabulated for a variety of loop operators, like the plaquette, in [9].) Note that R_1 communicates the lattice's violation of Lorentz invariance, and is therefore responsible for the bad behavior of the static potential, while R_2 and R_3 are Lorentz invariant. If we want to eliminate the $\mathcal{O}(a^2)$ lattice artifacts then we need to form an improved action by adding other Wilson loops to the action, which will give canceling amounts of R_1, R_2, R_3 .

Only R_1 contributes in Eq. (1) at tree-level, but quantum corrections bring in the other two operators. To remove all three, it might seem that we need to add three new Wilson loops to cancel these terms, but actually the coefficient of R_3 can be set to zero by a change of field variable in the path

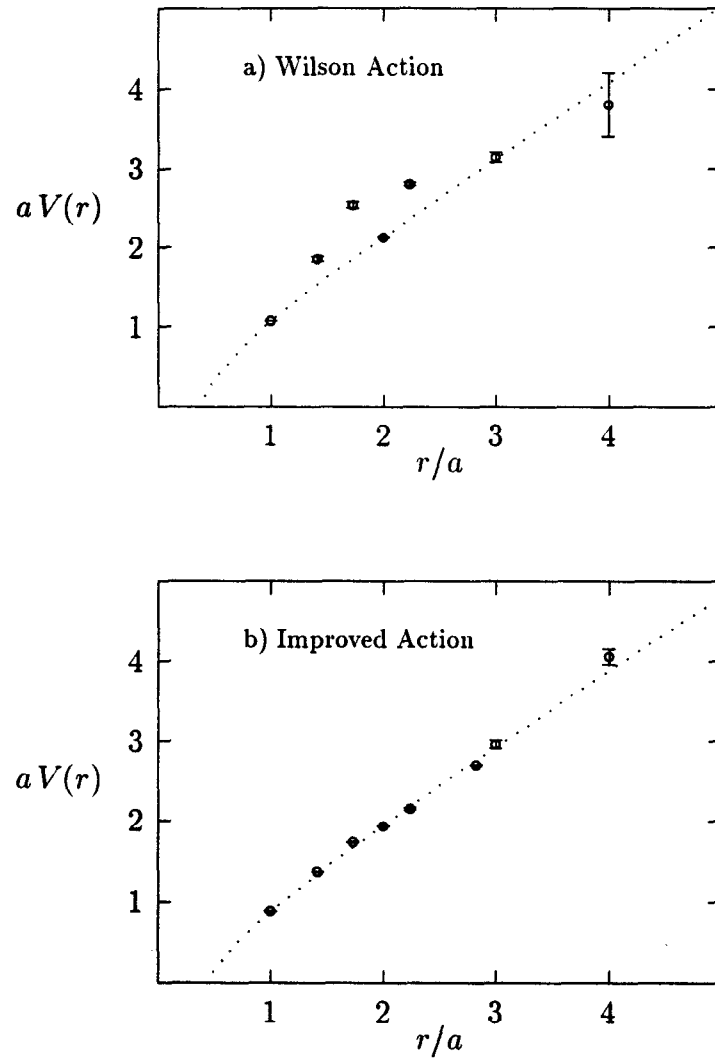


Figure 1: Static-quark potential computed on 6⁴ lattices with $a \approx 0.4$ fm using the $\beta = 4.5$ Wilson action and the improved action with $\beta_{\text{pl}} = 6.8$.

integral,

$$A_\mu \rightarrow A_\mu + a^2 \alpha_s f(\alpha_s) \sum_\nu D_\nu F_{\nu\mu}, \quad (3)$$

so only two new terms are needed [10, 9]. There are many possible choices for these, but we take the rectangle and “parallelogram”:

$$U_{\text{rt}} = \begin{array}{c} \text{---} \rightarrow \\ \text{---} \rightarrow \\ \leftarrow \text{---} \\ \leftarrow \text{---} \end{array} , \quad U_{\text{pg}} = \begin{array}{c} \text{---} \rightarrow \\ \text{---} \rightarrow \\ \text{---} \rightarrow \\ \leftarrow \text{---} \end{array} . \quad (4)$$

The improved action is [10, 9]

$$\begin{aligned} S[U] &= \beta_{\text{pl}} \sum_{\text{pl}} \frac{1}{3} \text{Re Tr}(1 - U_{\text{pl}}) \\ &+ \beta_{\text{rt}} \sum_{\text{rt}} \frac{1}{3} \text{Re Tr}(1 - U_{\text{rt}}) \\ &+ \beta_{\text{pg}} \sum_{\text{pg}} \frac{1}{3} \text{Re Tr}(1 - U_{\text{pg}}), \end{aligned} \quad (5)$$

with β_{pl} given as an input, and β_{rt} and β_{pg} computed in tadpole-improved perturbation theory to cancel out the $\mathcal{O}(a^2)$ terms in the derivative expansion of the action. At tree-level, the β 's are readily computed by combining expansions like Eq. (1) for each of the three loops. They are tadpole-improved by dividing each Wilson loop with L links by $(u_0)^L$ [3]. One-loop corrections have also been computed [11], but must be adjusted to account for the tadpole improvement. We find:

$$\beta_{\text{rt}} = -\frac{\beta_{\text{pl}}}{20 u_0^2} (1 + 0.4805 \alpha_s), \quad (6)$$

$$\beta_{\text{pg}} = -\frac{\beta_{\text{pl}}}{u_0^2} 0.03325 \alpha_s. \quad (7)$$

Following [3], we use the measured expectation value of the plaquette to determine both the value of the mean link u_0 and the QCD coupling constant α_s ,

$$u_0 = \left(\frac{1}{3} \text{Re Tr} \langle U_{\text{pl}} \rangle \right)^{1/4}, \quad (8)$$

$$\alpha_s = -\frac{\ln \left(\frac{1}{3} \text{Re Tr} \langle U_{\text{pl}} \rangle \right)}{3.06839}. \quad (9)$$

This result follows from the tree-level perturbative calculation of the plaquette [12]. The couplings β_{rt} and β_{pg} are determined self-consistently with u_0 and α_s for a given β_{pl} . As in NRQCD, there is no tuning of the couplings for the correction terms: tadpole-improved perturbation theory determines them in terms of the single bare coupling β_{pl} . Using identities from [9] we find that our action is positive semidefinite at least for $\beta_{\text{pl}} \geq 6.8$, which is necessary if perturbation theory is to be reliable.

The perturbative expansion (6) for β_{rt} already demonstrates the power of tadpole improvement. If one omits the tadpole factor u_0^2 , the expression becomes $\beta_{\text{rt}} = -\beta_{\text{pl}}(1 + 2.0 \alpha_s)/20$. Note that the coefficient of the one-loop-term α_s has quadrupled. Tadpole improvement automatically supplies 75% of the one-loop contribution needed without improvement. Since $\alpha_s \approx 0.3$, the unimproved expansion is not particularly convergent. However, with tadpole improvement, the one-loop correction is only about 10–20% of β_{rt} .

As indicated above, our improved action is not unique. Our techniques should work as well for actions with other forms for the correction terms. To verify this, we compare results obtained using our improved action above with those obtained from a tree-level improved action with a very different correction term [13]:

$$S_{\text{trt}}[U] = \beta_{\text{pl}} \sum_{\text{pl}} \frac{1}{3} \text{Re Tr}(1 - U_{\text{pl}}) + \beta_{\text{trt}} \sum_{\text{trt}} \frac{1}{3} \text{Re Tr}(1 - U_{\text{trt}}), \quad (10)$$

where U_{trt} is a twisted rectangle operator,

$$U_{\text{trt}} = \begin{array}{c} \square \quad \square \\ \diagup \quad \diagdown \end{array} . \quad (11)$$

At tree-level, with tadpole improvement,

$$\beta_{\text{trt}} = \frac{\beta_{\text{pl}}}{12 u_0^4}. \quad (12)$$

Note that tadpole improvement introduces four powers of u_0 here, rather than the two powers in β_{rt} above. This makes S_{trt} much more sensitive to tadpole improvement.

Action	β_{pl}	$\langle \frac{1}{3} \text{Re Tr } U_{\text{pl}} \rangle$	a	dimensions
improved	6.8	.46	.40 fm	$6^4, 6^3 \times 9$
	7.1	.506	.33 fm	$7^3 \times 10$
	7.4	.56	.24 fm	$8^3 \times 10, 9^3 \times 12$
S_{irt}	4.1	.454	.40 fm	$6^3 \times 9$
Wilson	4.5	.34	.40 fm	6^4
	5.7	.55	.17 fm	$12^3 \times 24, 16^4$

Table 1: Parameters used in our simulations. The additional couplings for improved actions were determined using the values listed in the table for β_{pl} and the plaquette.

3 Monte-Carlo Results

We conducted simulations with improved actions for a range of large lattice spacings (Table 1). The static-quark potential computed using our improved gluon action and the coarsest lattice is shown in Fig. 1b. As in the Wilson case (Fig 1a), the lattice spacing is about 0.4 fm. The dashed line in these plots is the standard infrared parameterization for the continuum potential, $V(r) = Kr - \pi/12r + c$, adjusted to fit the on-axis values of the potential. Off-axis points deviate from the fit by 40% for the Wilson theory, indicating a significant failure of rotation invariance due to finite- a errors. By contrast, the deviations are only 2–4% for the improved theory — negligible for most low-energy applications.

To assess the relative importance of tree-level improvement, tadpole improvement and one-loop corrections we computed the potential for several different actions, all with lattice spacings of about 0.4 fm. We focused on the deviation ΔV of $V(a, a, a)$ from the continuum potential adjusted to fit on-axis values of the simulated potential. ΔV is a sensitive indicator of violations of rotational invariance. Our results are in Table 2. As expected, the correction term in the action is significantly underestimated without tadpole improvement. The tadpole-improved action is very accurate both

Action	$\Delta V(\sqrt{3}a)/K\sqrt{3}a$
unimproved (Wilson)	0.41(2)
tree-level improved, no tadpole improvement	0.15(1)
one-loop improved, no tadpole improvement	0.12(2)
tree-level improved, with tadpole improvement	0.05(1)
one-loop improved, with tadpole improvement	0.04(1)
twisted-rectangle correction, with tadpole improvement	0.04(2)

Table 2: Error in the static quark potential at $V(a, a, a)$ for a variety of gluon actions. The lattice spacing in each case is $a \approx 0.4$ fm; K is the slope of the linear part of the static potential.

with and without one-loop corrections, suggesting that $\mathcal{O}(a^2\alpha_s)$ corrections are comparable to those of $\mathcal{O}(a^4)$.

We have also included in Table 2 results obtained using the twisted-rectangle action S_{trt} (10). We find that this action gives a potential that is essentially identical to that obtained with our other improved action. Note that tadpole improvement more than doubles the size of the correction term in S_{trt} when $a = 0.4$ fm. The quality of the results obtained from S_{trt} is strong evidence in support of tadpole improvement.

In computing the potentials, we assumed that the static quark propagator is simply the product of link operators $U_\mu(x)$ along the time axis. Our action is designed so that this is true at tree level through $\mathcal{O}(a^2)$, however there are corrections of order $\alpha_s a^2$. These arise because of the field transformation in Eq. (3). Our potential therefore has errors of $\mathcal{O}(\alpha_s a^2)$, even though the action is accurate up to errors of $\mathcal{O}(\alpha_s^2 a^2, a^4)$. Note that these particular errors in our potential do not break rotational invariance and so have no effect on the values of ΔV in Table 2. A straightforward perturbative calculation is needed to remove the $\mathcal{O}(\alpha_s a^2)$ errors from our potential.

To further check on our improved theory, we examined the spin-averaged

spectrum of the ψ family of mesons using NRQCD for the c -quarks and our improved action at $\beta_{\text{pl}} = 6.8, 7.1$ and 7.4 . Because we were examining only the spin-averaged spectrum, we omitted all spin-dependent corrections from the NRQCD action, but kept the corrections for $\mathcal{O}(a, a^2)$ errors, and for spin-independent $\mathcal{O}(v^2/c^2)$ effects [6]. The spectra, normalized to give the correct $1P$ - $1S$ splitting, are shown in Fig. 3 together with experimental results (dashed lines) and simulation results obtained using the Wilson action for the gluons at smaller a 's [6]. All agree to within 30–40 MeV. (The $2S$ simulation masses are a little above the true mass, which is expected since the simulation does not include light-quark loops.)

In Fig. 2 we show simulation results for the Coulomb-gauge radial wavefunctions of $1S$ and $1P$ charmonium as computed with the improved action on our coarsest and finest lattices. We also show wavefunctions computed from a continuum quark model tuned to reproduce our lattice results. The wavefunctions from the different lattice spacings agree well everywhere except at $r = 0$, where agreement is not expected (because of renormalization effects). The wavefunctions show remarkable radial symmetry considering that the rms radius of the $1S$ wavefunction, for example, is just 0.37 fm, or slightly less than one lattice spacing on the coarse lattice—accurate modeling of a hadron is possible with improved actions even when the hadron is only a few lattice spacings in extent.

We also calculated the ratio of the $1P$ - $1S$ charmonium splitting to the square root of the slope V' of the static potential at $r = 0.6$ fm [14]; our results are in Table 3. (We choose 0.6 fm because we have good simulation results for $V(r)$ at that radius and, also, V' is almost independent of r there.) This ratio is a dimensionless quantity that should become independent of lattice spacing as we approach the continuum limit. We see that, to within our errors, the improved action has reached the continuum limit at a lattice spacing of 0.4 fm, whereas the Wilson action has not. The twisted-rectangle action also gives excellent results at this lattice spacing.

Since coarse lattices have far fewer sites and much less critical-slowing-down, the cost to produce a statistically independent configuration should be much less on a coarser lattice. To examine this issue, we compared our results for $V(r)$ with those in [15] which are for the potential computed using the Wilson action at $\beta = 6$ (32^4 lattice with $a \approx 0.1$ fm). We rescaled the coordinates and potential from this other study to put them in the same units as our $\beta_{\text{pl}} = 6.8$ results, and examined the potentials

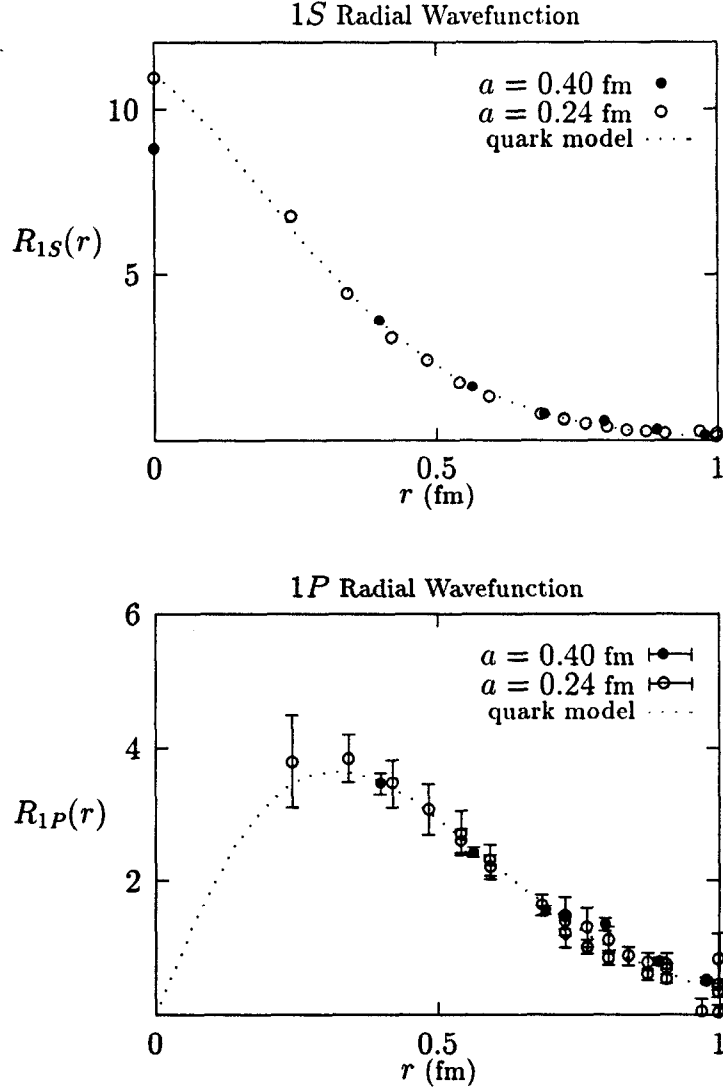


Figure 2: The radial wavefunctions for the $1S$ and $1P$ charmonium computed using improved actions and two different lattice spacings. Wavefunctions from a continuum quark model are also shown. Statistical errors are negligible for the $1S$ wavefunction.

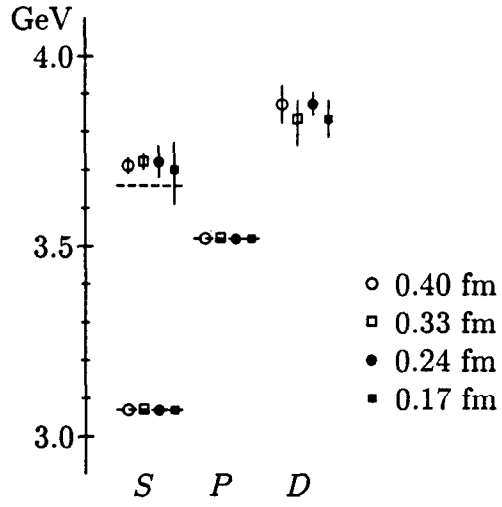


Figure 3: S , P , and D states of charmonium computed on lattices with: $a = 0.40$ fm (improved action, $\beta_{\text{pl}} = 6.8$); $a = 0.33$ fm (improved action, $\beta_{\text{pl}} = 7.1$); $a = 0.24$ fm (improved action, $\beta_{\text{pl}} = 7.4$); and $a = 0.17$ fm (Wilson action, $\beta = 5.7$). The dashed lines indicate the true masses.

Action	β_{pl}	a	$(1P - 1S)/\sqrt{V'}$
Wilson	4.5	.41 fm	1.38 (5)
	5.7	.17 fm	0.87 (3)
Improved	6.8	.40 fm	0.90 (1)
	7.1	.33 fm	0.92 (1)
	7.4	.24 fm	0.89 (2)
S_{trt}	4.1	.40 fm	0.92 (3)

Table 3: Ratio of the charmonium $1P - 1S$ splitting to the square root of the derivative of the static potential $V(r)$ at 0.6 fm.

at comparable distances. The results from both simulations are listed in Table 4. In both cases the potential is obtained from the time dependence of loop-like correlation functions for times equal to or larger than some T_{min} . Results should become independent of T_{min} once it is sufficiently large; with our much smaller statistical errors, we can measure the small shift when T_{min} is doubled from .4 fm to .8 fm. Our results required 1.3×10^7 site updates, while the analysis on the fine lattice required 6.4×10^9 site updates. Since statistical errors (for $T_{\text{min}} = 0.4$ fm) are about 20 times smaller for the coarse lattice, we estimate that comparable errors with the fine lattice would require 197,000 times more site updates than we used on the coarse lattice.

4 Conclusions

We have found that, by using perturbatively-improved action with tadpole-improved operators, we can accurately simulate quark and gluon dynamics on lattices with a spacing as large as 0.4 fm. Using either of two very different improved gluon actions, we obtained results for the confining potential and for charmonium that are independent of lattice-spacing artefacts to within a few percent.

It is striking that we can obtain accurate results on such coarse

r/a_c	$a = a_c = 0.40$		$a = 0.10$
	$T_{\min} = .4$	$T_{\min} = .8$	$T_{\min} = .3$
1	0.871 (0)	0.887 (1)	
0.962			0.839 (11)
$\sqrt{2}$	1.373 (1)	1.384 (2)	
1.361			1.316 (25)
$\sqrt{3}$	1.718 (2)	1.742 (10)	
1.667			1.581 (54)
2	1.897 (2)	1.941 (10)	
1.924			1.842 (42)

Table 4: Comparison of the static-quark potential $aV(r)$ as computed on a coarse lattice (improved action, $\beta_{\text{pl}} = 6.8$, $a = 0.40$ fm), and on a fine lattice (Wilson action, $\beta = 6$, $a = 0.10$ fm). T_{\min} is the shortest time interval used in the correlation functions that determine $V(r)$. All times and distances are in fm.

lattices using relatively simple actions. Following the ideas of the Wilson renormalization group, one expects, even at fixed, finite lattice spacing, to achieve arbitrarily accurate results by adding more and more operators to the discretized action, and by calculating their coefficients with increasing accuracy. We find that including just the leading corrections, with coefficients calculated in (tadpole-improved) tree-level perturbation theory, gives excellent results even on our coarsest lattices. Ultimately, nonperturbative calculations (for example, using Monte Carlo renormalization group methods) should be used to determine the coefficients, at least as a check of the perturbation theory. Such nonperturbative determinations of the couplings in the lattice action would be very interesting, although we expect such an effort to be much more difficult than the tadpole-improvement program outlined in this paper, and to produce only small changes to the coefficients determined here. In [3], the normalization of the strong coupling constant and the leading gluonic operator ($F_{\mu\nu}^2$) was carefully studied. We found that tadpole-improved perturbation theory gave normalizations that were extremely close to the nonperturbatively obtained

normalization.

The coarseness of the lattice makes our simulations 10^4 – 10^5 times faster than ones using unimproved actions; in fact, most of the $a = 0.4$ fm results in this paper were obtained using an IBM RS6000/250 desktop workstation, which is powered by a personal-computer CPU (66MHz PowerPC). We therefore believe that, using the methods we have described, the QCD hadron spectrum can be calculated to an accuracy of a few percent using computer resources that are already widely available. And by combining these techniques with forefront computing technology, we can begin to tackle problems in nonperturbative QCD far more complex than previously imagined.

Acknowledgments

We are very grateful to A. Pierce, IBM, and Cornell's Center for Theory and Simulation for help in using their IBM SP-2 supercomputer for our larger calculations. Some calculations in this work were performed on the Fermilab lattice supercomputer, ACPMAPS. This work was supported by the DOE and NSF.

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